The Burnett expansion of the periodic Lorentz gas

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Abstract

Recently, stretched exponential decay of multiple correlations in the periodic Lorentz gas has been used to show the convergence of a series of correlations which has the physical interpretations as the fourth order Burnett coefficient, a generalization of the diffusion coefficient. Here the result is extended to include all higher order Burnett coefficients, and give a plausible argument that the expansion constructed from the Burnett coefficients has a finite radius of convergence.

1 Introduction

The *Lorentz gas* is a model used in statistical mechanics, consisting of a point particle moving at constant velocity except for specular collisions with smooth (specifically C^3) convex fixed scatterers in $d \geq 2$ dimensions. The original model [8] has randomly placed scatterers in infinite space, and is thought to have power law decay of correlations, so that the Burnett coefficients (defined below as sums of such correlations) are not generally expected to exist [6, 11]. Here we consider a periodic arrangement of scatterers which is equivalent to a dispersing billiard on a torus, for which it is known that two-time correlations of the discrete (collision) dynamics decay exponentially [4, 12]. This, together with the *finite horizon* condition, that is, that the time between collisions is bounded, implies the existence of the diffusion coefficient ($D^{(2)}$ below).

A recent paper gives a stretched exponential decay of multiple correlations [5], and uses this to show (again with finite horizon) that the fourth order Burnett coefficient ($D^{(4)}$ below) exists. Here we extend this result to all the Burnett coefficients. A common example for $d = 2$ with a finite horizon is given by circular scatterers on a triangular lattice; for $d > 2$ the finite horizon condition requires either nonspherical scatterers, or more than one scatterer per unit cell. The Lorentz gas and a number of extensions are discussed in Ref. [10].

The Burnett coefficients $D^{(m)}$ discussed in this paper are defined using series of correlation functions. Section 2 defines these series and gives three basic results about them.

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Section 3 gives the main result of this paper, the proof of convergence of these series. The series arise in a physical description of diffusion, however the derivation involves hydrodynamic approximations and interchange of limits which have not been justified rigorously for the Lorentz gas. The physical motivation together with the non-rigorous derivation of the series given below from previously stated formulas is given in the final section, together with a conjecture about the Burnett expansion.

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2 Definitions

In the following, $\boldsymbol{\phi}(x)$ is the billiard map defined on the collision space M, consisting of points $x = (\mathbf{r}, \mathbf{v}) \in M$ for which the position $\mathbf{r} \in \mathbb{R}^d$ is on the boundary of one of the scatterers and the velocity following a collision $\mathbf{v} \in \mathbb{R}^d$ is of unit magnitude in an outward direction from the scatterer. Greek indices $\alpha, \beta, \ldots = 1, \ldots, d$ denote components of vectors and tensors in $\mathbb{R}^d$, and a dot $\mathbf{a} \cdot \mathbf{b}$ denotes the usual inner product $\sum_\alpha a_\alpha b_\alpha$ corresponding to the Euclidean metric. We have two functions $T : M \to \mathbb{R}$ and $\mathbf{a} : M \to \mathbb{R}^d$ which describe the embedding of the collision dynamics into physical space and time, as follows. $T(x)$ is the time (also distance since the speed of the particle is one) between the collision at x and the next; it is a piecewise Hölder continuous function [1, 3]. $\mathbf{a}(x)$ is the lattice translation vector associated with this free flight when the configuration variable $\mathbf{r}$ is unfolded onto a periodic tiling of $\mathbb{R}^d$; it is a linear combination of the lattice basis vectors $\mathbf{e}^{(\alpha)}$ with integer coefficients, and is a piecewise constant function. The finite horizon condition ensures that both T and $\mathbf{a}$ are bounded. The average $\langle \cdot \rangle$ denotes integration over M with respect to the invariant equilibrium measure. In terms of this average we define $\Delta T : M \to \mathbb{R}$ by $\Delta T(x) = T(x) - \langle T \rangle$ so that $\langle \Delta T \rangle = 0$.

The billiard dynamics is time reversal invariant, that is, there exists an involution $\mathcal{T} : M \to M$ (given simply by the specular reflection law) with the property

$$\boldsymbol{\phi} \circ \mathcal{T} \circ \boldsymbol{\phi} = \mathcal{T} \tag{1}$$

In addition, $\mathcal{T}$ preserves the equilibrium measure, that is,

$$\langle \mathcal{T} \circ g \rangle = \langle g \rangle \tag{2}$$

for arbitrary measurable function $g : M \to M$. The map $\mathcal{T}$ also satisfies

$$T \circ \mathcal{T} \circ \boldsymbol{\phi} = T \tag{3}$$

$$\mathbf{a} \circ \mathcal{T} \circ \boldsymbol{\phi} = -\mathbf{a} \tag{4}$$

Thus $\langle \mathbf{a} \rangle = 0$.

The wave vector $\mathbf{k}$ is to be understood as a formal real expansion parameter with d components (although physically we would like to interpret it as a vector with a value in $\mathbb{R}^d$). The *dispersion relation* $s[\mathbf{k}]$ is to be understood as a formal power series

$$s[\mathbf{k}] = \sum_{m=2}^{\infty} \imath^m \sum_{\alpha_1 \ldots \alpha_m} D^{(m)}_{\alpha_1 \ldots \alpha_m} k_{\alpha_1} \ldots k_{\alpha_m} \tag{5}$$

in terms of the *Burnett coefficients* $D^{(m)}$ which are assumed to be real, totally symmetric tensors of rank m. That is, an equation (specifically Eq. (15) below) involving $s[\mathbf{k}]$ is to be interpreted as a sequence of equations (specifically Eq. (16) below) obtained by equating coefficients of powers of $\mathbf{k}$. The symbol $\imath$ denotes $\sqrt{-1}$.

The existence of Burnett coefficients satisfying the equations (16) is not assumed a priori; we show in Lemma 1 below that equations (16) express the $d(d+1)/2$ independent components of $D^{(2)}$ as series not containing any of the $D^{(m)}$, then the $d(d+1)(d+2)/6$ independent components of $D^{(3)}$ as series containing only the $D^{(2)}$ and so on. Lemma 2 shows that they are indeed real, and Thm. 4 shows that the limit exists.

We define formal power series f and F by

$$f[\mathbf{k}] \equiv s[\mathbf{k}]\Delta T + \imath \mathbf{k} \cdot \mathbf{a} \tag{6}$$

$$F[\mathbf{k}] \equiv \sum_{i=-n}^{n-1} f[\mathbf{k}] \circ \boldsymbol{\phi}^i \tag{7}$$

where the dependence on x and on the positive integer n is suppressed in the notation; the limit $n \to \infty$ will be taken later. We have $\langle f \rangle = 0$ and $\langle F \rangle = 0$ at each order in $\mathbf{k}$ and for each n as a consequence of $\langle \Delta T \rangle = 0$ and $\langle \mathbf{a} \rangle = 0$ above.

We define *cumulants* $Q_N[\mathbf{k}]$ (also formal power series) for integers $N \geq 2$ as

$$Q_N[\mathbf{k}] = \sum_{\{\nu_j\}: \sum_j j\nu_j = N} (-1)^{\nu-1} \frac{(\nu-1)! \prod_j \langle F[\mathbf{k}]^j \rangle^{\nu_j}}{\prod_j (\nu_j! j!^{\nu_j})} \tag{8}$$

with j and ν_j integers satisfying $j \geq 2$ and $\nu_j \geq 0$, and $\nu = \sum_j \nu_j$ is the total number of correlations in the product. For example

$$\begin{aligned} Q_2 &= \langle F^2 \rangle / 2 && (9) \\ Q_3 &= \langle F^3 \rangle / 6 && (10) \\ Q_4 &= (\langle F^4 \rangle - 3\langle F^2 \rangle^2)/24 && (11) \\ Q_5 &= (\langle F^5 \rangle - 10\langle F^3 \rangle \langle F^2 \rangle)/120 && (12) \\ Q_6 &= (\langle F^6 \rangle - 15\langle F^4 \rangle \langle F^2 \rangle - 10\langle F^3 \rangle^2 + 30\langle F^2 \rangle^3)/720 && (13) \end{aligned}$$

Now Q_N contains exactly N powers of F, and so it contains terms $\mathbf{k}^m$ only for $m \geq N$, and we can write it as

$$Q_N[\mathbf{k}] = \sum_{m=N}^{\infty} \sum_{\alpha_1 \ldots \alpha_m} q_{N,m;\alpha_1 \ldots \alpha_m} k_{\alpha_1} \ldots k_{\alpha_m} \tag{14}$$

thus defining totally symmetric tensors $q_{N,m}$ for $m \geq N$.

The Burnett coefficients are found by equating the formal power series on both sides of

$$s[\mathbf{k}] = \lim_{n\to\infty} \frac{1}{2n\langle T\rangle} \sum_{N=2}^{\infty} Q_N[\mathbf{k}] \tag{15}$$

that is,

$$\imath^m D^{(m)}_{\alpha_1\ldots\alpha_m} = \lim_{n\to\infty} \frac{1}{2n\langle T\rangle} \sum_{N=2}^{m} q_{N,m;\alpha_1\ldots\alpha_m} \tag{16}$$

These equations determine the $D^{(m)}$ explicitly as real tensors, subject to convergence of the limit, as shown by the following two lemmas.

Lemma 1 *The right hand side of Eq. (16) does not contain $D^{(m')}$ such that $m' \geq m$.*

Proof: We have $N \geq 2$, and each Q_N contains N powers of F, thus each term has at least 2 powers of F. Each F has at least 1 power of $\mathbf{k}$, and there are m powers of $\mathbf{k}$ in total, so each F has at most $m-1$ powers of $\mathbf{k}$. $D^{(m')}$ appear in F associated with m' powers of $\mathbf{k}$, so $m' \leq m-1$ for any $D^{(m')}$ appearing.

Remark: It is possible there are no factors of $D^{(m')}$ on the right hand side, in fact the lemma shows that this is true for $m=2$. The case $m=2$ can easily be written explicitly; Eq. (16) becomes

$$D^{(2)}_{\alpha\beta} = \lim_{n\to\infty} \frac{1}{4n\langle T\rangle} \sum_{i=-n}^{n-1} \sum_{j=-n}^{n-1} \langle a^i_\alpha a^j_\beta\rangle \tag{17}$$

This is a discrete time version of the well-known Green-Kubo formula for the diffusion tensor (which reduces to a single diffusion coefficient in the isotropic case $D^{(2)}_{\alpha\beta} = D\delta_{\alpha\beta}$). An equivalent discrete time equation appears in [7], also for $m=4$.

Lemma 2 *Despite the appearance of the imaginary number $\imath$ in the above definitions, the Burnett coefficients are real if they exist.*

Proof: We note from the definitions that $s[\mathbf{k}]$, $f[\mathbf{k}]$ and $F[\mathbf{k}]$ have pure imaginary coefficients for odd powers of $\mathbf{k}$ and real coefficients for even powers of $\mathbf{k}$. This property is preserved by addition and multiplication of power series, so it also holds for the $Q_N[\mathbf{k}]$. This implies that the $q_{N,m}$ are imaginary for odd m and real for even m. The result follows from Eq. (16).

Before proceeding with the more technical convergence proof, we note another important result:

Lemma 3 *$D^{(m)} = 0$ for m odd.*

Proof: From the properties of the time reversal operator $\mathcal{T}$ given above, $\langle F^j\rangle$ has zero contribution from any term with an odd number of $\mathbf{a}$ factors. The result follows by induction on m: assume that $D^{(m')} = 0$ for all odd $m' < m$, then by Lemma 1 all terms in $s[\mathbf{k}]$ contributing to $D^{(m)}$ have even powers of $\mathbf{k}$, and from the oddness of $\mathbf{a}$ under time reversal, so also do the $\imath\mathbf{k}\cdot\mathbf{a}$ terms. Thus $D^{(m)}$, which is constructed from terms with m powers of $\mathbf{k}$, must be zero for m odd.

3 Convergence of the series

The averages $\langle F^j \rangle$ appearing in the cumulants contain summations over j variables with range $-n$ to $n-1$, and could grow as fast as $O(n^j)$ in general. Thus each term, which is a product of such averages could grow as $O(n^N)$ in general. For the limit in Eq. (16) to exist, we require that the series grows only as $O(n)$. Although the growth of each product of correlations cannot be controlled this well, cancellations occur in constructing the cumulants. This is expressed in the following theorem which, together with Lemmas 1 and 2, implies the existence of the Burnett coefficients:

Theorem 4 *$q_{N,m}$ is defined in Eqs. (7, 8, 14) for integers N and m satisfying $2 \leq N \leq m$. The limit*

$$\lim_{n\to\infty} \frac{1}{n} q_{N,m;\alpha_1\ldots\alpha_m} \tag{18}$$

exists for all such N and m in the periodic Lorentz gas.

The structure of the proof of Thm. 4 is as follows. We state the theorem expressing stretched exponential decay of multiple correlation functions. Next, the terms appearing in (16) are written as a time ordered sum, so that this theorem can be applied. Then we show that all the terms connected by the application of the theorem have coefficients which sum to zero, so that only the stretched exponential corrections remain. Finally, a bound of n multiplied by a polynomial is put on the number of terms at each order of the stretched exponential, so that the series divided by n converges absolutely.

Thm. 4 is based on the following result:

Theorem 5 *(Theorem 2 of Ref. [5]) Let $i_1 \leq \cdots \leq i_k$ and $1 \leq t \leq k-1$. Then*

$$|\langle f_1^{i_1} \cdots f_k^{i_k} \rangle - \langle f_1^{i_1} \cdots f_t^{i_t} \rangle \langle f_{t+1}^{i_{t+1}} \cdots f_k^{i_k} \rangle| \leq C_k \cdot |i_k - i_1|^2 \lambda^{|i_{t+1}-i_t|^{1/2}} \tag{19}$$

where $C_k > 0$ depends on the functions $f_1, \ldots, f_k$, and $\lambda < 1$ is independent of k and $f_1, \ldots, f_k$.

The theorem applies to piecewise Hölder continuous functions f_j such that $\langle f_j \rangle = 0$ for all j and uses notation $f_j^i \equiv f_j \circ \boldsymbol{\phi}^i$. As noted in Ref. [5], we expect based on Refs. [12, 4] that it should be possible to prove a stronger bound $\lambda^{|i_{t+1}-i_t|}$, but the above bound is sufficient for our purposes here.

The $q_{N,m}$ as defined in the previous section are finite sums of terms of the form (see Eqs. (7, 8, 14))

$$\sum_{\{\nu_j\}:\sum_j j\nu_j = N} (-1)^{\nu-1} \frac{(\nu-1)!}{\prod_j (\nu_j! j!^{\nu_j})} \sum_{i_1\ldots i_N=-n}^{n-1} \langle f_1^{i_1} \ldots f_j^{i_j} \rangle \langle f_{j+1}^{i_{j+1}} \ldots \rangle \ldots \langle \ldots f_N^{i_N} \rangle \tag{20}$$

multiplied by constants such as the lower order Burnett coefficients. The f here and for the remainder of this section are T or $\mathbf{a}$, both of which satisfy the conditions of Thm. 5.

The exact number of terms of this kind is not important; it depends on N and m but not n and therefore does not affect convergence of the limit $n \to \infty$.

In order to use Thm. 5 we need to put the times i_p in numerical order. The unrestricted sum over all the i_p is replaced by an ordered sum $i_1 \leq i_2 \ldots i_N$ over all $N!/S[i]$ permutations of the i_p. $S[i]$ is a symmetry factor to account for the fact that some of the i_p may be equal; the exact form is unimportant since it is a common prefactor, independent of the ν_j. Not all $N!$ permutations of the correlations are distinct: it does not matter in which order the f_j are multiplied within a correlation, or which order correlations of equal numbers of f_j are multiplied; thus both factorials in the denominator disappear, leading to

$$\sum_{\{\nu_j\}:\sum_j j\nu_j=N} (-1)^{\nu-1}(\nu-1)! \left[\sum_{i_1\leq i_2\ldots i_N} \frac{1}{S[i]} \left\{\langle f_1^{i_1}\ldots f_j^{i_j}\rangle\langle f_{j+1}^{i_{j+1}}\ldots\rangle\ldots\langle\ldots f_N^{i_N}\rangle \right.\right.$$
$$\left.\left. + \text{ permutations}\right\}\right] \tag{21}$$

The "permutations" remaining in (21) consist of the remaining $N!/(\prod_j \nu_j! j!^{\nu_j}) - 1$ rearrangements of the i_p that are not equivalent by reordering the product of correlations or the product of f within a correlation.

As an example, we give the expression for $N = 6$:

$$\begin{aligned}
&\sum_{i_1\leq i_2\leq i_3\leq i_4\leq i_5\leq i_6} \frac{1}{S[i]} \Big\{\langle f_1^{i_1} f_2^{i_2} f_3^{i_3} f_4^{i_4} f_5^{i_5} f_6^{i_6}\rangle \\
&-\Big[\langle f_1^{i_1} f_2^{i_2}\rangle\langle f_3^{i_3} f_4^{i_4} f_5^{i_5} f_6^{i_6}\rangle + \langle f_1^{i_1} f_3^{i_3}\rangle\langle f_2^{i_2} f_4^{i_4} f_5^{i_5} f_6^{i_6}\rangle + \langle f_1^{i_1} f_4^{i_4}\rangle\langle f_2^{i_2} f_3^{i_3} f_5^{i_5} f_6^{i_6}\rangle \\
&+\langle f_1^{i_1} f_5^{i_5}\rangle\langle f_2^{i_2} f_3^{i_3} f_4^{i_4} f_6^{i_6}\rangle + \langle f_1^{i_1} f_6^{i_6}\rangle\langle f_2^{i_2} f_3^{i_3} f_4^{i_4} f_5^{i_5}\rangle + \langle f_2^{i_2} f_3^{i_3}\rangle\langle f_1^{i_1} f_4^{i_4} f_5^{i_5} f_6^{i_6}\rangle \\
&+\langle f_2^{i_2} f_4^{i_4}\rangle\langle f_1^{i_1} f_3^{i_3} f_5^{i_5} f_6^{i_6}\rangle + \langle f_2^{i_2} f_5^{i_5}\rangle\langle f_1^{i_1} f_3^{i_3} f_4^{i_4} f_6^{i_6}\rangle + \langle f_2^{i_2} f_6^{i_6}\rangle\langle f_1^{i_1} f_3^{i_3} f_4^{i_4} f_5^{i_5}\rangle \\
&+\langle f_3^{i_3} f_4^{i_4}\rangle\langle f_1^{i_1} f_2^{i_2} f_5^{i_5} f_6^{i_6}\rangle + \langle f_3^{i_3} f_5^{i_5}\rangle\langle f_1^{i_1} f_2^{i_2} f_4^{i_4} f_6^{i_6}\rangle + \langle f_3^{i_3} f_6^{i_6}\rangle\langle f_1^{i_1} f_2^{i_2} f_4^{i_4} f_5^{i_5}\rangle \\
&+\langle f_4^{i_4} f_5^{i_5}\rangle\langle f_1^{i_1} f_2^{i_2} f_3^{i_3} f_6^{i_6}\rangle + \langle f_4^{i_4} f_6^{i_6}\rangle\langle f_1^{i_1} f_2^{i_2} f_3^{i_3} f_5^{i_5}\rangle + \langle f_5^{i_5} f_6^{i_6}\rangle\langle f_1^{i_1} f_2^{i_2} f_3^{i_3} f_4^{i_4}\rangle\Big] \\
&-\Big[\langle f_1^{i_1} f_2^{i_2} f_3^{i_3}\rangle\langle f_4^{i_4} f_5^{i_5} f_6^{i_6}\rangle + \langle f_1^{i_1} f_2^{i_2} f_4^{i_4}\rangle\langle f_3^{i_3} f_5^{i_5} f_6^{i_6}\rangle + \langle f_1^{i_1} f_2^{i_2} f_5^{i_5}\rangle\langle f_3^{i_3} f_4^{i_4} f_6^{i_6}\rangle \\
&+\langle f_1^{i_1} f_2^{i_2} f_6^{i_6}\rangle\langle f_3^{i_3} f_4^{i_4} f_5^{i_5}\rangle + \langle f_1^{i_1} f_3^{i_3} f_4^{i_4}\rangle\langle f_2^{i_2} f_5^{i_5} f_6^{i_6}\rangle + \langle f_1^{i_1} f_3^{i_3} f_5^{i_5}\rangle\langle f_2^{i_2} f_4^{i_4} f_6^{i_6}\rangle \\
&+\langle f_1^{i_1} f_3^{i_3} f_6^{i_6}\rangle\langle f_2^{i_2} f_4^{i_4} f_5^{i_5}\rangle + \langle f_1^{i_1} f_4^{i_4} f_5^{i_5}\rangle\langle f_2^{i_2} f_3^{i_3} f_6^{i_6}\rangle + \langle f_1^{i_1} f_4^{i_4} f_6^{i_6}\rangle\langle f_2^{i_2} f_3^{i_3} f_5^{i_5}\rangle \\
&+\langle f_1^{i_1} f_5^{i_5} f_6^{i_6}\rangle\langle f_2^{i_2} f_3^{i_3} f_4^{i_4}\rangle\Big] \qquad\qquad (22) \\
&+2\Big[\langle f_1^{i_1} f_2^{i_2}\rangle\langle f_3^{i_3} f_4^{i_4}\rangle\langle f_5^{i_5} f_6^{i_6}\rangle + \langle f_1^{i_1} f_2^{i_2}\rangle\langle f_3^{i_3} f_5^{i_5}\rangle\langle f_4^{i_4} f_6^{i_6}\rangle + \langle f_1^{i_1} f_2^{i_2}\rangle\langle f_3^{i_3} f_6^{i_6}\rangle\langle f_4^{i_4} f_5^{i_5}\rangle \\
&+\langle f_1^{i_1} f_3^{i_3}\rangle\langle f_2^{i_2} f_4^{i_4}\rangle\langle f_5^{i_5} f_6^{i_6}\rangle + \langle f_1^{i_1} f_3^{i_3}\rangle\langle f_2^{i_2} f_5^{i_5}\rangle\langle f_4^{i_4} f_6^{i_6}\rangle + \langle f_1^{i_1} f_3^{i_3}\rangle\langle f_2^{i_2} f_6^{i_6}\rangle\langle f_4^{i_4} f_5^{i_5}\rangle \\
&+\langle f_1^{i_1} f_4^{i_4}\rangle\langle f_2^{i_2} f_3^{i_3}\rangle\langle f_5^{i_5} f_6^{i_6}\rangle + \langle f_1^{i_1} f_4^{i_4}\rangle\langle f_2^{i_2} f_5^{i_5}\rangle\langle f_3^{i_3} f_6^{i_6}\rangle + \langle f_1^{i_1} f_4^{i_4}\rangle\langle f_2^{i_2} f_6^{i_6}\rangle\langle f_3^{i_3} f_5^{i_5}\rangle \\
&+\langle f_1^{i_1} f_5^{i_5}\rangle\langle f_2^{i_2} f_3^{i_3}\rangle\langle f_4^{i_4} f_6^{i_6}\rangle + \langle f_1^{i_1} f_5^{i_5}\rangle\langle f_2^{i_2} f_4^{i_4}\rangle\langle f_3^{i_3} f_6^{i_6}\rangle + \langle f_1^{i_1} f_5^{i_5}\rangle\langle f_2^{i_2} f_6^{i_6}\rangle\langle f_3^{i_3} f_4^{i_4}\rangle \\
&+\langle f_1^{i_1} f_6^{i_6}\rangle\langle f_2^{i_2} f_3^{i_3}\rangle\langle f_4^{i_4} f_5^{i_5}\rangle + \langle f_1^{i_1} f_6^{i_6}\rangle\langle f_2^{i_2} f_4^{i_4}\rangle\langle f_3^{i_3} f_5^{i_5}\rangle + \langle f_1^{i_1} f_6^{i_6}\rangle\langle f_2^{i_2} f_5^{i_5}\rangle\langle f_3^{i_3} f_4^{i_4}\rangle\Big]\Big\}
\end{aligned}$$

Here, the four terms correspond to the partitions of 6 which do not contain 1; in the above notation the nonzero ν_j are $\{\nu_6 = 1\}$ with $6!/6! = 1$ term; $\{\nu_2 = 1, \nu_4 = 1\}$ with

$6!/2!4! = 15$ terms; $\{\nu_3 = 2\}$ with $6!/2!3!^2 = 10$ terms; and $\{\nu_2 = 3\}$ with $6!/3!2!^3 = 15$ terms; compare with Eq. (13).

Now we apply Thm. 5 to the largest gap, $i_{t+1} - i_t$. Any of the largest gaps will suffice if more than one is largest. Before tackling the general case, we see how it works in the $N = 6$ example. Notice that, whatever the value of t, the theorem combines all the above correlations to leave terms (the number of which is a function of N) bounded by $\lambda^{|i_{t+1}-i_t|^{1/2}}$ multiplied by powers of the time differences. Explicitly, for $t = 1$, all terms cancel individually because $\langle f_j\rangle = 0$. For $t = 2$ the $\langle f^6\rangle$ term cancels with one of the $\langle f^2\rangle\langle f^4\rangle$ terms, six other $\langle f^2\rangle\langle f^4\rangle$ terms cancel with three of the $\langle f^2\rangle^3$ terms and the remaining terms all split leaving an $\langle f\rangle$ term. For $t = 3$ the $\langle f^6\rangle$ term cancels with one of the $\langle f^3\rangle^2$ terms, and all of the others split leaving an $\langle f\rangle$ term. $t = 4$ is analogous to $t = 2$ and $t = 5$ is analogous to $t = 1$.

In general we must show that the coefficient $(-1)^{\nu-1}(\nu-1)!$ in Eq. (21) combined with the numbers of terms of various types leads to complete cancellation for all values of N. Consider a general term (ignoring the $S[i]$ which is the same for each term) which is *unaffected* by a split at time t. Each correlation contains times $i_p \le t$ or times $i_p > t$ but not both. Thus it can be written schematically as

$$\langle\rangle\langle\rangle\ldots\langle\rangle|\langle\rangle\langle\rangle\ldots\langle\rangle \tag{23}$$

where all times i_p to the left of the bar "|" are less than or equal to t and all times to the right of the bar are greater than t. Let there be A correlations to the left and B correlations to the right, so $A + B = \nu$.

This term will cancel (up to stretched exponential corrections) with any term which is split to the same form, if the sum of the coefficients (the $(-1)^{\nu-1}(\nu-1)!$) is zero. The terms that are split to a given form consist of correlations that are either the same as the above, or are joined in a pairwise fashion with a correlation on the other side of the bar.

Again, an example is helpful: When $N = 8$, a split at $t = 4$ combines the following terms: $-6\langle f_1^{i_1} f_2^{i_2}\rangle\langle f_3^{i_3} f_4^{i_4}\rangle|\langle f_5^{i_5} f_6^{i_6}\rangle\langle f_7^{i_7} f_8^{i_8}\rangle$ with $2\langle f_1^{i_1} f_2^{i_2} f_5^{i_5} f_6^{i_6}\rangle\langle f_3^{i_3} f_4^{i_4}\rangle\langle f_7^{i_7} f_8^{i_8}\rangle$, $2\langle f_1^{i_1} f_2^{i_2} f_7^{i_7} f_8^{i_8}\rangle\langle f_3^{i_3} f_4^{i_4}\rangle\langle f_5^{i_5} f_6^{i_6}\rangle$, $2\langle f_1^{i_1} f_2^{i_2}\rangle\langle f_3^{i_3} f_4^{i_4} f_5^{i_5} f_6^{i_6}\rangle\langle f_7^{i_7} f_8^{i_8}\rangle$, $2\langle f_1^{i_1} f_2^{i_2}\rangle\langle f_3^{i_3} f_4^{i_4} f_7^{i_7} f_8^{i_8}\rangle\langle f_5^{i_5} f_6^{i_6}\rangle$, $-\langle f_1^{i_1} f_2^{i_2} f_5^{i_5} f_6^{i_6}\rangle\langle f_3^{i_3} f_4^{i_4} f_7^{i_7} f_8^{i_8}\rangle$ and $-\langle f_1^{i_1} f_2^{i_2} f_7^{i_7} f_8^{i_8}\rangle\langle f_3^{i_3} f_4^{i_4} f_5^{i_5} f_6^{i_6}\rangle$. These all cancel because $-6 + 2 + 2 + 2 + 2 - 1 - 1 = 0$.

The term given in Eq. (23) has coefficient $(-1)^{\nu-1}(\nu-1)!$. There are AB terms with coefficient $(-1)^{\nu-2}(\nu-2)!$ obtained by combining a single correlation on the left and the right. There are $A(A-1)B(B-1)/2!$ terms with coefficient $(-1)^{\nu-3}(\nu-3)!$ obtained by combining two correlations on the left and the right, and so on until all $\min(A, B)$ correlations on the side with the fewest correlations have been combined. The total coefficient is thus given by

$$H(A,B) \equiv \sum_{p=0}^{\min(A,B)} (-1)^{A+B-p-1}(A+B-p-1)!\frac{A!B!}{(A-p)!(B-p)!p!} \tag{24}$$

To show that the coefficients cancel, we therefore need the following lemma:

Lemma 6 *$H(A,B)=0$ for all positive integers A and B.*

Proof: The sum is symmetric in A and B so suppose that $A \geq B$ without loss of generality. Then the summand is the product of a constant $(-1)^{A+B-1}A!$, an alternating binomial of degree B, that is, $(-1)^{-p}B!/((B-p)!p!)$ and a polynomial in p of degree $B-1$, that is, $(A+B-p-1)!/(A-p)!$. We will use summation by parts to lower the degree of both until the result is zero.

We note the summation by parts formula

$$\sum_{p=0}^{B} x_p y_p = y_0 \sum_{p=0}^{B} x_p + \sum_{q=1}^{B}(y_q - y_{q-1}) \sum_{p=q}^{B} x_p \tag{25}$$

which can be demonstrated by collecting terms on the right hand side. Now substituting $x_p = (-1)^{-p}B!/((B-p)!p!$ and $y_p = (A+B-p-1)!/(A-p)!$ we can show by induction on q from B downwards that

$$\sum_{p=q}^{B} x_p = \begin{cases} (-1)^{-q}\frac{(B-1)!}{(B-q)!(q-1)!} & q>0 \\ 0 & q=0 \end{cases} \tag{26}$$

hence the first term on the right hand side of Eq. (25) vanishes. We can also simplify

$$y_q - y_{q-1} = (1-B)\frac{(A+B-q-1)!}{(A-q+1)!} \tag{27}$$

so Eq. (24) now reads

$$H(A,B) = (-1)^{A+B-1}A!(1-B)\sum_{q=1}^{B} \frac{(-1)^{-q}(B-1)!}{(B-p)!(p+1)!}\frac{(A+B-q-1)!}{(A-q+1)!} \tag{28}$$

Shifting the summation index by one we find

$$H(A,B) = (1-B)H(A,B-1) \tag{29}$$

The proof of Lemma 6 follows by noting that $H(A,1)=0$.

We now conclude the proof of Thm. 4. Recall that the series (20) have been rewritten in the form (21). Thm. 5 is applied to (one of) the largest gap(s) $\Delta i_{\max} \equiv i_{t+1} - i_t$, partitioning the terms into subsets which split into a particular form (23). Lemma 6 shows that the coefficients of all terms in a subset conspire to cancel, so that each subset is bounded by the error term in theorem 5, that is $\lambda^{|\Delta i_{\max}|^{1/2}}$ multiplied by a polynomial in the time differences.

Finally we estimate the number of terms with each value of $\Delta i_{\max}$. The first time i_1 varies freely from $-n$ to $n-1$, having a total of $2n$ values. One of the time differences is equal to $\Delta i_{\max}$, and the other $k-2$ time differences can range from 0 to $\Delta i_{\max}$, so the total number of terms with a given $\Delta i_{\max}$ is less than $2n(k-1)\Delta i_{\max}^{(k-2)}$, in particular a polynomial in $\Delta i_{\max}$ multiplied by n. Thus the series divided by n appearing in Thm. 4 is bounded by a product of polynomial factors and the decaying stretched exponential, and hence converges absolutely. This concludes the proof of Thm. 4 and the proof of existence of Burnett coefficients.

4 Physical motivation and remarks

This section makes the connection between the Burnett coefficients defined in the previous sections and equations found in the physics literature. The latter equations are phenomenological and have not been shown rigorously in a limiting fashion from the Lorentz gas, and a few nonrigorous limit interchanges are made to connect them with the expressions defined in the previous sections. First we consider the dispersion relation, the equation for the Burnett coefficients, and finally the whether the dispersion relation can be used to define an analytic function.

The dispersion relation (5) with $\mathbf{k}$ interpreted as a real vector represents the solution of a generalised diffusion equation proposed by Burnett [2] containing higher derivative terms that become important on small scales,

$$\partial_t \rho = \sum_{m=2}^{\infty} \sum_{\alpha_1 \ldots \alpha_m} D^{(m)}_{\alpha_1 \ldots \alpha_m} \partial_{\alpha_1} \ldots \partial_{\alpha_m} \rho \tag{30}$$

assuming a solution of the form

$$\rho(\mathbf{r}, t) \sim \exp(s(\mathbf{k})t + \imath \mathbf{k} \cdot \mathbf{r}) \tag{31}$$

Here, $\partial_\alpha \equiv \partial / \partial r_\alpha$. Nonlinear terms such as powers of $\partial_\alpha \rho$ are excluded on physical grounds since ρ is a projection onto real space ($\mathbf{r} \in \mathbb{R}^d$) of a phase space density satisfying a linear evolution equation. The *phase space* is a subset of $\mathbb{R}^{2dM}$ corresponding to the possible positions and velocities of $M \gg 1$ particles. The dispersion relation is a more robust formulation than the generalized diffusion equation (30) since the former may be supplemented by nonanalytic functions of $\mathbf{k}$ to account for situations (other than the periodic Lorentz gas) in which some of the Burnett coefficients do not exist.

Chapter 7 of Ref. [7] obtains the dispersion relation from the microscopic dynamics using the equation (7.91 in this reference):

$$1 = \lim_{n \to \infty} \langle \prod_{i=-n}^{n-1} \exp[-s(\mathbf{k}) T(\boldsymbol{\phi}^i x) - \imath \mathbf{k} \cdot \mathbf{a}(\boldsymbol{\phi}^i x)] \rangle \tag{32}$$

We write $T = \langle T \rangle + \Delta T$ as in previous sections, take out the constant factor of $\langle T \rangle$, and take the logarithm to find

$$s(\mathbf{k}) = \lim_{n \to \infty} \frac{1}{2n \langle T \rangle} \ln \langle \exp[F(\mathbf{k})] \rangle \tag{33}$$

where F is defined (as a power series) in Eq. (7). Now the exponential and the logarithm are expanded in power series and the resulting terms containing N powers of F are collected to become the cumulants Q_N defined in Eq. (8). The cumulant form of the expansion is possibly more robust than the above equations due to the cancellations among the terms that combine to construct each cumulant.

Since it is desirable from a physical point of view to interpret $\mathbf{k}$ as a real variable, we conclude with the following conjecture:

Conjecture 7 *The series (5) converges when* $\mathbf{k} \in \mathcal{D} \subset \mathbb{R}^d$ *for some nontrivial domain* $\mathcal{D}$*, and so defines a function* $s(k)$ *in this domain.*

Note that $s(k)$ (if it exists) is a real function as a consequence of Lemma 3, and physically is expected to be negative except at the origin (otherwise the density ρ would grow exponentially with time); this puts further constraints on the Burnett coefficients.

Unfortunately the proof given in the previous section contains many undetermined functions of $\mathbf{k}$, and the Burnett coefficients are defined by a complicated recursive relation (16), so a proof is unlikely using the techniques of this paper.

There are two results that make such a result plausible. The first is that in the Boltzmann limit of a hard sphere gas, that is, a gas with many moving particles at low density and with recollisions ignored, the expansion in $\mathbf{k}$ (in this context called the linearized Chapman-Enskog expansion) converges [9]. Of course, the hard sphere collisions are similar to that of the Lorentz gas, but recollisions cannot be ignored in general.

The second result is exact, but for a highly simplified (piecewise linear) system. We consider the map $\boldsymbol{\phi} : \mathbb{R} \to \mathbb{R}$ given by

$$\boldsymbol{\phi}(x) = \frac{3}{2} - 2x + 3[x] \tag{34}$$

where $[x]$ is the greatest integer less than or equal to x. The dynamics defined by $\boldsymbol{\phi}$ is equivalent to a random walk where the particle moves with equal probability from one interval $I_n \equiv (n - 1/2, n + 1/2)$ to the left, I_{n-1} or to the right, I_{n+1}. The dispersion relation $s(k)$ follows directly from the above phenomenological solution (31),

$$\rho(n, t) = \exp(st + ikn) \tag{35}$$

After one iteration,

$$\begin{aligned} \rho(n, 1) &= \frac{1}{2}[\exp(\imath k(n-1)) + \exp(\imath k(n+1))] && (36) \\ &= \cos k \exp(\imath kn) && (37) \end{aligned}$$

leading to

$$s(k) = \ln \cos k \tag{38}$$

which has a power series around $k = 0$ with a radius of convergence equal to $\pi/2$.

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